Escape problem for irreversible systems

Robert S. Maier
Department of Mathematics, University of Arizona, Tucson, Arizona 85721

D. L. Stein
Department of Physics, University of Arizona, Tucson, Arizona 85721
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The problem of noise-induced escape from a metastable state arises in physics, chemistry, biology, systems engineering, and other areas. The problem is well understood when the underlying dynamics of the system obey detailed balance. When this assumption fails many of the results of classical transition-rate theory no longer apply, and no general method exists for computing the weak-noise asymptotic behavior of fundamental quantities such as the mean escape time. In this paper we present a general technique for analyzing the weak-noise limit of a wide range of stochastically perturbed continuous-time nonlinear dynamical systems. We simplify the original problem, which involves solving a partial differential equation, into one in which only ordinary differential equations need be solved. This allows us to resolve some old issues for the case when detailed balance holds. When it does not hold, we show how the formula for the asymptotic behavior of the mean escape time depends on the dynamics of the system along the most probable escape path. We also present results on short-time behavior and discuss the possibility of *focusing* along the escape path.

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I. INTRODUCTION

The phenomenon of escape from a locally stable equilibrium state arises in a multitude of scientific contexts [1–3]. If a nonlinear system is subjected to continual random perturbations ("noise"), eventually a sufficiently large fluctuation will drive it over an intervening barrier to a new equilibrium state. The mean amount of time required for this to occur typically grows exponentially as the strength of the random perturbations tends to zero.

Research on this phenomenon has focused on the case when the nonlinear dynamics of the system in the absence of random perturbations are specified by a *potential function*. In a recent paper [4] we have introduced an alternative technique for computing the weak-noise asymptotic behavior of the mean first-passage time (MFPT) to the barrier. Our technique, unlike the bulk of earlier work, is not restricted to the case when the zero-noise dynamics arise from a potential. Because of this we can readily and quantitatively treat systems without "detailed balance," whose dynamics are determined by nongradient drift fields, or are otherwise time irreversible. We deal here with *overdamped* systems, in which inertia plays no role. Overdamped systems without detailed balance arise in the theory of glasses and other disordered materials [5], chemical reactions far from equilibrium [6], stochastically modeled computer networks [7–9], evolutionary biology [10], and theoretical ecology [11].

In the multidimensional escape problems most frequently considered in the literature, the most probable escape path (MPEP) in the limit of weak noise passes over a saddle point of the unperturbed dynamics. In the case of nongradient drift fields exit through an *unstable* equilibrium point can also occur [4]. Other possibilities, such as exit through a limit cycle [12, 13], arise as well. However, if the unperturbed dynamics are determined by a potential, exit in the limit of weak noise must occur over a saddle point, and the asymptotic behavior of the MFPT is given by a classic formula, originally derived in the context of chemical reactions by Eyring [14].

Over the years the Eyring formula has been rederived and generalized by a variety of alternative approaches [15–17]. To illustrate its use, consider a two-dimensional system whose dynamics are specified by a sufficiently smooth drift field $\mathbf{u} = \mathbf{u}(x, y)$ symmetric about the x axis as displayed in Fig. 1. $S = (x_S, 0)$ and $H = (0, 0)$ denote the stable equilibrium point and saddle point, and the barrier lies along the y axis. The position of a point particle representing the system state, moving in this drift field and subjected to additive white noise $\dot{\mathbf{w}}(t)$, satisfies the Itô stochastic differential equation [18]

$$dx_i(t) = u_i(\mathbf{x}(t))\, dt + \epsilon^{1/2}\sigma_i\, dw_i(t), \quad i = x, y. \qquad (1)$$

Here σ_x and σ_y quantify the response of the particle to the perturbations in the x and y directions; the corresponding diffusion tensor $\mathbf{D}$ is $\mathrm{diag}(D_x, D_y) = \mathrm{diag}({\sigma_x}^2, {\sigma_y}^2)$ and will in general be anisotropic. If the drift field $\mathbf{u}$ is obtained from a potential function $\phi = \phi(x, y)$ by the formula $u_i = -D_i\partial_i\phi$ then $\mathbf{u}$ will in general not be a gradient field, but the relation between $\mathbf{u}$ and $\mathbf{D}$ will ensure detailed balance [19].

If detailed balance holds, the Eyring formula for the $\epsilon \to 0$ asymptotic behavior of the MFPT τ is

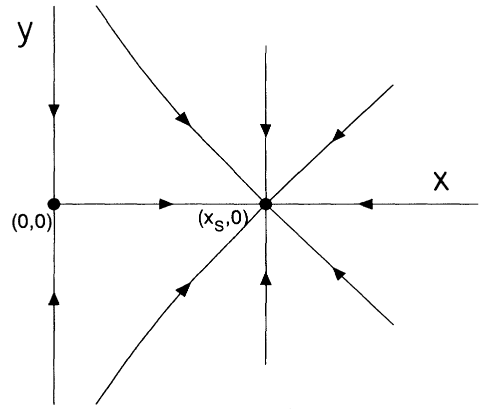

FIG. 1. A drift field $\mathbf{u}$ symmetric about the x axis, with stable equilibrium point $S = (x_S, 0)$ and saddle point $H = (0,0)$. $\lambda_x(S)$ and $\lambda_y(S)$, the eigenvalues of the linearization of $\mathbf{u}$ at S, are taken to be real and negative. This sketch assumes $\lambda_x(S) = \lambda_y(S)$, but that is not assumed in the text.

$$\frac{1}{\tau} \sim \frac{1}{\pi}\sqrt{\left|\frac{\partial u_x}{\partial x}(S)\right|\frac{\partial u_x}{\partial x}(H)}\sqrt{\frac{(\partial u_y/\partial y)(S)}{(\partial u_y/\partial y)(H)}} \times \exp\left[-\frac{2}{D_x\epsilon}\int_0^{x_S} dx\; u_x(x,0)\right], \qquad (2)$$

where $(\partial u_y/\partial y)(S)$ is $\partial u_y/\partial y$ evaluated at the stable point S, and $(\partial u_y/\partial y)(H)$ is $\partial u_y/\partial y$ evaluated at the saddle point H, etc. In this example the MPEP lies along the x axis; this fact was used implicitly in the expression for the Arrhenius (i.e., exponential) factor in (2). If the vector field were asymmetric and the MPEP were curved, the Arrhenius factor would involve the integral $\int(\mathbf{D}^{-1}\mathbf{u})\cdot d\mathbf{x}$ taken along the MPEP [20].

Equation (2) displays a frequently encountered feature of weak-noise escape problems: the dependence on $\mathbf{u}$ of the preexponential factor in the asymptotic behavior of the MFPT is limited to a dependence on the derivatives of $\mathbf{u}$ near the stable equilibrium and saddle points. If detailed balance is absent this will generally not be the case [21, 22]. However, most quantitative work on the case when detailed balance is absent has dealt with one-dimensional state spaces, due to the difficulty of higher-dimensional computations. Talkner and Hänggi [23] computed the asymptotic behavior of the MFPT for a multidimensional model of an optically bistable system without detailed balance, in which the drift field did not arise from a potential. But due to the simplicity of their model, the prefactor did not display a complicated dependence on the drift. Multidimensional models without detailed balance have not been treated in full generality.

In Secs. II and III we start from scratch and compute the weak-noise asymptotic behavior of the MFPT for multidimensional systems by singular perturbation methods, using matched asymptotic expansions. Similar approaches have been used before [12, 24], but our treatment yields a systematic method of computing the preexponential factor, even in cases when detailed balance is absent. As noted, we have previously applied our techniques to the nonclassical case of exit over an *unstable* equilibrium point (i.e., an equilibrium point at which the linearization of $\mathbf{u}$ has only positive eigenvalues) [4]. The MFPT asymptotic behavior differed considerably from the classical escape formulas such as Eq. (2); the prefactor in the asymptotic behavior of τ depended on ϵ. In this paper we flesh out the ideas in our previous paper by applying them to drift fields with the standard structure of Fig. 1. We discover that even when the MPEP passes over a saddle point, if detailed balance is absent the asymptotic behavior of the MFPT likewise differs from that given by the Eyring formula. Although the prefactor is independent of ϵ, it depends on the behavior of $\mathbf{u}$ along the entire MPEP. We quantify this dependence; it can be much more complicated than a dependence on the derivatives of $\mathbf{u}$ at the endpoints.

Our treatment reveals, however, that when $\mathbf{u}$ is symmetric about the MPEP as displayed in Fig. 1 the prefactor can readily be computed by integrating two coupled ordinary differential equations along the MPEP. Previous work has left the impression that partial differential equations must be solved. In the absence of detailed balance, the asymptotic behavior of the MFPT is determined by a *quasipotential* [25], the solution of a nonlinear partial differential equation. However, the derivatives of this function along the MPEP, which turn out to determine the prefactor, satisfy ordinary differential equations.

The prefactor is very sensitive to the behavior of the drift field in a neighborhood of the MPEP. Integrating the ordinary differential equations along the MPEP requires knowledge of the extent of "differential shearing" along the MPEP, i.e., knowledge of the second derivatives of $\mathbf{u}$ there. In many cases differential shearing can give rise to a *focusing singularity* along the MPEP, in which case more sophisticated techniques must be used.

When detailed balance is absent, both the short-term dynamics of the system and the asymptotic behavior of the MFPT display novel behavior in the limit of weak noise. As noted, the system fluctuates around the locally stable equilibrium state many times before it finally escapes along the MPEP. If the drift field $\mathbf{u}$ arises from a potential, each of the unsuccessful escape attempts follows an outward "instanton" trajectory antiparallel to some integral curve of $\mathbf{u}$ and then falls back along the same integral curve (an "anti-instanton" trajectory). In the absence of detailed balance, the time irreversibility will generally cause the instanton trajectories *not* to be antiparallel to the anti-instanton trajectories, which remain integral curves of the drift field. Hence unsuccessful escape attempts will proceed with high probability along closed *loops* containing nonzero area, in contrast to the more familiar situation for systems with detailed balance. We discuss this in Sec. IV; conclusions appear in Sec. V.

II. THE ANALYSIS

We now derive the weak-noise asymptotic behavior of the MFPT for any $\mathbf{u}$ with the general structure of Fig. 1, but not necessarily derived from a potential. We allow anisotropic diffusion, so long as the principal axes of the diffusion tensor are aligned with the MPEP. After approximating the probability density of the system along the MPEP, we will compute τ by the Kramers method of computing the probability flux through the separatrix, i.e., the boundary of the basin of attraction of the stable point.

The Fokker-Planck equation for the probability density ρ is $\dot{\rho} = \mathcal{L}^* \rho$, with

$$\mathcal{L}^* = (\epsilon/2)(D_x \partial_x^2 + D_y \partial_y^2) - u_x(x,y)\partial_x - u_y(x,y)\partial_y - \partial_x u_x(x,y) - \partial_y u_y(x,y). \quad (3)$$

If absorbing boundary conditions are imposed on the separatrix (in this case, the y axis), the MFPT in the weak-noise limit may be approximated by $(-\lambda_1)^{-1}$, where λ_1 is the eigenvalue of the slowest decaying density mode ρ_1 (i.e., the eigenfunction of $\mathcal{L}^*$ whose eigenvalue has the greatest real part). λ_1 is negative and converges to zero as $\epsilon \to 0$, so in the weak-noise limit $(-\lambda_1)^{-1}$ displays Arrhenius growth. We have

$$-\lambda_1 = \frac{\int_{-\infty}^{\infty} (D_x \epsilon/2) \partial_x \rho_1(0,y)\, dy}{\int_0^{\infty} \int_{-\infty}^{\infty} \rho_1(x,y)\, dy\, dx} \quad (4)$$

since the right-hand side is the normalized flux of probability through the separatrix. The leading asymptotic behavior of λ_1, as computed by this formula, will be unaffected [12] if ρ_1 is taken to satisfy $\mathcal{L}^* \rho_1 = 0$.

According to (4), to approximate λ_1 we must approximate the normal derivative of ρ_1 along the separatrix. But since the MPEP passes through a saddle point, the probability density will be concentrated in a small region [of size $O(\epsilon^{1/2})$] about this point as $\epsilon \to 0$. It therefore suffices to approximate ρ_1 near the saddle point. To evaluate the denominator of (4), we must also approximate ρ_1 near the stable point. The latter approximation is straightforward: near $(x_S, 0)$ we take

$$\rho_1(x,y) \sim \exp\{-[D_x^{-1}|\lambda_x(S)|(x-x_S)^2 + D_y{}^{-1}|\lambda_y(S)|y^2]/\epsilon\}, \quad (5)$$

where we now write $\lambda_x(S)$, $\lambda_y(S)$, $\lambda_x(H)$, and $\lambda_y(H)$ for the (real) eigenvalues of the drift field linearized at the stable and saddle points, respectively. This Gaussian approximation permits the evaluation of the denominator of (4). It is $\pi\epsilon\sqrt{D_x D_y}/\sqrt{\lambda_x(S)\lambda_y(S)} + o(\epsilon)$, since contributions from other regions are negligible.

It remains to approximate ρ_1 in the vicinity of the saddle point. As a necessary first step, we approximate ρ_1 along the MPEP, i.e., the x axis. In the vicinity of the MPEP we use a standard WKB approximation

$$\rho_1(x,y) \sim K(x,y)\exp[-W(x,y)/\epsilon]. \quad (6)$$

Here W is the quasipotential, the "nonequilibrium potential" investigated by Graham and others [26, 27]. K satisfies a transport equation, and W an eikonal (Hamilton-Jacobi) equation: $H(\mathbf{x}, \nabla W) = 0$, with H the Wentzell-Freidlin Hamiltonian [25]

$$H(\mathbf{x},\mathbf{p}) = \frac{D_x}{2}p_x^2 + \frac{D_y}{2}p_y^2 + \mathbf{u}(\mathbf{x}) \cdot \mathbf{p}. \quad (7)$$

So $W(x,y)$ can be viewed as the classical action of the zero-energy trajectory from $(x_S, 0)$ to (x,y). If detailed balance holds, i.e., $u_i = -D_i \partial_i \phi$ for some potential function ϕ, it is easily checked that $W(x,y) = 2\phi(x,y) + C$, where C is an arbitrary constant. If detailed balance is absent then W will in general be more difficult to compute. The zero-energy classical trajectories determined by the Hamiltonian of (7) include the instanton trajectories; we will return to this point in Sec. IV.

Given the drift-field structure shown in Fig. 1, and assuming sufficient smoothness, we can expand $\mathbf{u}$ near the x axis in powers of y,

$$u_x = v_0(x) + v_2(x)y^2 + O(y^4), \quad (8)$$

$$u_y = u_1(x)y + O(y^3). \quad (9)$$

Using this notation, we have, e.g., $\lambda_y(S) = u_1(x_S)$ and $\lambda_x(H) = \partial v_0/\partial x(0)$. The function v_2 measures the extent of differential shearing along the MPEP.

Again assuming sufficient smoothness, we can expand W itself near the x axis in powers of y,

$$W(x,y) = f_0(x) + f_2(x)y^2 + O(y^4), \quad (10)$$

where $f_2(x)$ is a measure of the transverse behavior of the "WKB tube" of probability current along the MPEP; clearly, $f_2(x) = \frac{1}{2}\partial^2 W/\partial y^2(x,0)$. Physically, f_2 measures the transverse length scale on which the probability density is non-negligible. The tube profile will be approximately Gaussian, with variance proportional to $\epsilon/f_2(x)$ at position x.

Substituting the *Ansatz* (6) into $\mathcal{L}^*\rho_1 = 0$ and equating the coefficients of powers of ϵ yields a system of equations for the functions f_0, f_2, K in terms of v_0, v_2, u_1. (The system closes: no higher derivatives of $\mathbf{u}$ or W enter.) The first of these is the one-dimensional eikonal equation $H(x, f_0'(x)) = 0$, where

$$H(x,p_x) = \frac{D_x}{2}{p_x}^2 + v_0(x)p_x \quad (11)$$

is a Hamiltonian governing motion along the MPEP. For this Hamiltonian,

$$\dot{x} = D_x p_x + v_0(x) \quad (12)$$

is the expression relating velocity and momentum.

By the eikonal equation, $f_0'(x)$ can be viewed as the momentum p_x of an on-axis classical trajectory with zero energy. It follows from the Hamiltonian (11) that there are only two solutions to the eikonal equation: $f_0'(x) = -2v_0(x)/D_x$ [arising from an instanton trajectory moving against the drift, with $\dot{x} = -v_0(x)$], and $f_0 \equiv 0$ [arising from an anti-instanton trajectory following the drift, with $\dot{x} = +v_0(x)$]. That these trajectories are directly antiparallel to each other is a consequence of our assumption that the drift field is symmetric about the x-axis MPEP. Since physical exit trajectories begin at the stable point and terminate near the saddle point, when constructing the WKB approximation (6) we use the instanton solution $f_0'(x) = -2v_0(x)/D_x$ rather than the anti-instanton solution $f_0 \equiv 0$.

The equation for f_2 is a nonlinear Riccati equation, and may be written as

$$\dot{f}_2 = -2D_y f_2^2 - 2u_1 f_2 + 2v_0 v_2 / D_x, \tag{13}$$

where the dot signifies derivative with respect to instanton transit time. [Since the instanton trajectory satisfies $\dot{x} = -v_0(x)$, the left-hand side equals $-v_0 f_2'$.] This equation has an immediate physical interpretation: it describes how the WKB tube spreads out or contracts under the influence of its environment, as one progresses along the MPEP. The final inhomogeneous term on the right-hand side of (13) is particularly important. If the differential shearing v_2 is sufficiently negative in some portion of the MPEP, this term can drive f_2 to zero before the hyperbolic point is reached [4, 9]. If this occurs, to leading order the WKB tube splays out to infinite width. The tube width actually remains finite, but becomes larger than $O(\epsilon^{1/2})$; this becomes clear if higher-order terms are taken into account.

If f_2 goes negative, further integration of (13) will normally drive f_2 to $-\infty$ in finite time; for a pictorial example of this "focusing" phenomenon, which is really the appearance of a singularity in the nonequilibrium potential, see Fig. 1 of Day [28]. Equation (13) accordingly gives a quantitative measure of the validity of our WKB approximation: for it to be valid, f_2 must remain positive along the entire MPEP.

It has not been recognized that the validity of the WKB approximation along a straight MPEP can be so easily checked. Nonlinear equations resembling (13) have been derived by Schuss [18] and Talkner and Ryter [13, 29], but in the context of motion along the separatrix rather than along the MPEP. Their equations are homogeneous rather than inhomogeneous, so they give rise to no singularities. Ludwig and Mangel [24, 30] derived a homogeneous equation in the context of motion along an anti-instanton trajectory, i.e., motion following the drift.

The third and final equation is for the function K. The transport equation for $K(x,y)$ is a well-known partial differential equation [12, 13], but for the computation of the MFPT asymptotic behavior an ordinary differential equation along the MPEP will suffice. We may approximate K within the WKB tube as a function of x alone, in which case we find

$$\dot{K}/K = -u_1 - D_y f_2. \tag{14}$$

In the vicinity of the MPEP, the WKB approximation (6) arising from perturbations of the on-axis instanton trajectory $\dot{x} = -v_0(x)$ is completely determined by the ordinary differential equations (13) and (14), together with the initial conditions $f_2(x_S) = |\lambda_y(S)|/D_y$ and $K(x_S) = 1$. These follow from the requirement that the WKB approximation match the Gaussian approximation (5) near the stable point $(x_S, 0)$.

Finally we can approximate ρ_1 near the saddle point $H = (0,0)$. In the diffusion-dominated region within an $O(\epsilon^{1/2})$ distance of the origin, ρ_1 satisfies the equation

$$(\epsilon/2)(D_x \partial_x^2 \rho_1 + D_y \partial_y^2 \rho_1) - \partial_x(\lambda_x x \rho_1) - \partial_y(\lambda_y y \rho_1) = 0 \tag{15}$$

which is separable: $\rho_1(x,y) = \rho_1^x(x)\rho_1^y(y)$. By the symmetry of $\mathbf{u}$, ρ_1^y must be even; the absorbing boundary condition on the separatrix implies that ρ_1^x must be odd. The separation constant, and the overall normalization, are found by requiring that this solution match the WKB approximation (6).

For the matching to occur, the separation constant must equal zero. The symmetry requirements mandate that

$$\rho_1(x,y) \sim C e^{X^2/4} y_2(\tfrac{1}{2}, X) \exp[-|\lambda_y(H)| y^2 / D_y \epsilon]. \tag{16}$$

We have introduced the rescaled variable $X = x\sqrt{2\lambda_x(H)/D_x\epsilon}$, and $y_2(\frac{1}{2}, \cdot)$ is the odd parabolic cylinder function [31] of index $\frac{1}{2}$. $y_2(\frac{1}{2}, \cdot)$ can be expressed in terms of elementary functions, but we write ρ_1 in terms of it to facilitate comparison with our earlier work on exit over an unstable equilibrium point [4]. There a similar expression occurred, but the index of the parabolic cylinder function was not fixed. Compare the treatment of Caroli *et al.* [15], in whose treatment Weber functions (i.e., parabolic cylinder functions) of variable index were used. Note that $y_2'(\frac{1}{2}, 0) = 1$ by definition, and that $y_2(\frac{1}{2}, X) \sim \sqrt{\pi/2}\, e^{X^2/4}$ as $X \to +\infty$.

The normalization constant C is obtained by matching the $X \to +\infty$ asymptotic behavior of $\rho_1(x,y)$ to the WKB solution near the hyperbolic point. This gives

$$C = K(0)\sqrt{2/\pi}\, \exp\left[-\frac{2}{D_x\epsilon}\int_0^{x_S}, u_0(x)\, dx\right], \tag{17}$$

where $K(0)$ must be computed by integrating (14) along the MPEP from S to H. Since f_2 appears on the right-hand side of (14), this in turn requires an integration of (13) along the MPEP.

The essential point here is that the behavior of ρ_1 near the hyperbolic point — in particular, its overall normalization — can in general only be obtained by integrating along the MPEP, and will depend on the entire history of $\mathbf{u}$ and its first and second partial derivatives along it. Substituting our approximations (5) and (16) for ρ_1 into Eq. (4) now yields

$$\frac{1}{\tau} \sim \frac{K(0)}{\pi}\sqrt{|\lambda_x(S)|\lambda_x(H)}\sqrt{\frac{\lambda_y(S)}{\lambda_y(H)}} \times \exp\left[-\frac{2}{D_x\epsilon}\int_0^{x_S} u_0(x)\, dx\right], \tag{18}$$

which resembles the Eyring formula (2) but contains an additional "frequency factor" $K(0)$.

It can be shown that this formula for the small-ϵ asymptotic behavior of the MFPT is essentially equivalent to

$$\frac{1}{\tau} \sim \frac{\lambda_+}{\pi}\frac{\rho_0(H)}{\rho_0(S)}. \tag{19}$$

Equation (19) is a formula of Talkner [13], in which λ_+ is the (imaginary) frequency of the unstable mode of vibration at the saddle, and $\rho_0(S)$, $\rho_0(H)$ are proportional to the *stationary* probability densities at the stable point and the saddle which one would have if reflecting rather than absorbing boundary conditions were imposed on the separatrix. A similar formula appears in Schuss [18]. However, Eq. (19) does not indicate how $\rho_0(H)$ is to be found. Our treatment makes it clear that for drift fields with the structure of Fig. 1, the frequency factor $K(0)$ and the extent to which the MFPT asymptotic behavior differ from the Eyring formula are most easily computed by integrating the ordinary differential equations (13) and (14) along the MPEP.

III. EXPLICIT EXAMPLES

If the drift field is derived from a potential, we recover the Eyring formula as follows. As noted, if $u_i = -D_i\partial_i\phi$ for some potential function ϕ then $W(x,y) = 2\phi(x,y)$ up to an additive constant. This simplifies the calculation of f_2: the nonlinear Riccati equation for f_2 need not be integrated explicitly, though it could be. Necessarily

$$f_2(x) = \frac{1}{2}\frac{\partial^2 W(x,y)}{\partial y^2}\bigg|_{(x,0)} = \frac{\partial^2\phi(x,y)}{\partial y^2}\bigg|_{(x,0)} = -{D_y}^{-1}\frac{\partial u_y}{\partial y}\bigg|_{(x,0)} = -u_1(x)/D_y. \tag{20}$$

Equation (20) settles a recurring issue. It is sometimes assumed [15], in studying multidimensional escapes, that if $\mathbf{u}$ varies too rapidly along the MPEP the WKB approximation may break down due to f_2 going negative at some point along the MPEP. We have just shown that if detailed balance holds, *this will never happen*, so long as u_1 satisfies the obvious transverse stability condition of being strictly negative. In the language of chemical physics, that $f_2(x) = -u_1(x)/D_y$ for every x says that in this case, transverse fluctuations are in local thermal equilibrium at all points x along the MPEP. If detailed balance is lacking, $f_2(x)$ will not depend on $u_1(x)$ alone; Eq. (13) makes this observation quantitative.

It follows immediately from (14) and (20) that $K \equiv$ const; since $K(x_S) = 1$, $K(0) = 1$ also. So the formula (18) reduces to the Eyring formula when $\mathbf{u}$ is derived from a potential.

To illustrate the power of our technique, we now examine an overdamped system without detailed balance where the frequency factor $K(0)$ cannot be computed analytically. Suppose for simplicity that $D_x = D_y = 1$, and consider the drift field

$$u_x = x - x^3 - \alpha x y^2, \tag{21}$$

$$u_y = -y - x^2 y. \tag{22}$$

It is easily checked that this has the structure shown in Fig. 1 for any α, with $x_S = 1$, and that for $\alpha = 1$ (and only $\alpha = 1$) this $\mathbf{u}$ is derivable from a potential ϕ. In this case

$$\phi(x,y) = -\tfrac{1}{2}x^2 + \tfrac{1}{4}x^4 + \tfrac{1}{2}y^2 + \tfrac{1}{2}x^2y^2. \tag{23}$$

Note that for all α, the eigenvalues $\lambda_x(S) = -2$, $\lambda_y(S) = -2$, $\lambda_x(H) = 1$, and $\lambda_y(H) = -1$.

If $\alpha = 0$, u_x is independent of y and the escape time problem becomes essentially one dimensional. In particular, the asymptotic behavior of the MFPT is given by the one-dimensional Kramers formula [3]

$$\frac{1}{\tau} \sim \frac{1}{\pi}\sqrt{|\lambda_x(S)|\lambda_x(H)}\,\exp\left(-\frac{2}{\epsilon}\Delta\phi\right). \tag{24}$$

As α varies between zero and one, we expect the asymptotic behavior of τ to interpolate smoothly between the Kramers formula (24) and the Eyring formula (2).

Our technique can be used to solve for $K(0)$ and the prefactor in the MFPT asymptotic behavior for any value of α. In general, a numerical integration of the equations (13) and (14) for f_2 and K is required. Though this is straightforward, it is more illustrative of the value of our technique to perturb about the values of α at which analytic solutions can be obtained.

We therefore consider the drift field (21) and (22) with $\alpha = 1+\delta$, $|\delta| \ll 1$, and solve for the first-order (in δ) correction to $K(0)$ in (18). We have $u_1 = -(1+x^2)$, $v_0 = x - x^3$, and $v_2 = -(1+\delta)x$. Assuming sufficient smoothness, we expand f_2 in powers of δ,

$$f_2 = f_2^{(0)} + \delta f_2^{(1)} + o(\delta) = (1+x^2) + \delta f_2^{(1)} + o(\delta), \tag{25}$$

since $f_2^{(0)} = -u_1/D_y$ when $\alpha = 1$. Substituting this expansion into (13), we find a *linear* equation for the first-order correction $f_2^{(1)}$,

$$\frac{d}{dx}f_2^{(1)} = 2\left(\frac{1+x^2}{x-x^3}\right)f_2^{(1)} + 2x. \tag{26}$$

This inhomogeneous first-order equation is easily solved,

$$f_2^{(1)} = \frac{2x^2}{(1-x^2)^2}\left[\ln x + (1-x^2) + \tfrac{1}{4}(x^4-1)\right]. \tag{27}$$

Notice that when $\delta \neq 0$ and detailed balance is lacking, to first order $f_2(x)$ will differ from $-u_1(x)/D_y$ at all x along the MPEP. So if $\alpha \neq 1$, we expect that the transverse fluctuations are in local thermal equilibrium nowhere along the MPEP.

Using Eq. (11), and converting the derivative with respect to instanton transit time to a space derivative gives the equation for K,

$$K'/K = \delta\frac{2x}{(1-x^2)^3}\left(\ln x + \tfrac{3}{4} + \tfrac{1}{4}x^4 - x^2\right). \tag{28}$$

Its solution is

$$K(x)/K(1) = \exp\left(\frac{-\delta[1 - x^2 - (2x^4 - 4x^2)\ln x]}{4(1-x^2)^2}\right). \tag{29}$$

From this we find, to order δ, $K(0) = K(1)(1+\frac{3}{8}\delta) = 1+\frac{3}{8}\delta$. So

$$\frac{1}{\tau} \sim \frac{1+\frac{3}{8}\delta}{\pi}\sqrt{|\lambda_x(S)|\lambda_x(H)}\sqrt{\frac{\lambda_y(S)}{\lambda_y(H)}}\,\exp\left(-\frac{2}{\epsilon}\Delta\phi\right) \tag{30}$$

to first order in δ. Equation (30) displays the first-order correction to the Eyring asymptotic behavior.

Just as we have perturbed about the analytically soluble $\alpha = 1$ model, we could also perturb about the analytically soluble $\alpha = 0$ model, where detailed balance is altogether absent. When $\alpha = 0$ the nonequilibrium potential $W(x, y)$ cannot be computed explicitly. However, its transverse second derivative f_2 along the MPEP can be computed explicitly by integrating (13). The computation of the first-order correction $f_2^{(1)}$ yields corrections to the Kramers asymptotic behavior of (24); details are left to the reader.

Notice that since $v_2 = -\alpha x$, when α is sufficiently large and positive the function f_2 obtained by integrating the differential equation (13) along the MPEP will develop a zero at some point between $x = 1$ and $x = 0$. At this point the WKB tube will (naively, see Sec. II) splay out to infinite width, and the WKB approximation will break down. This is qualitatively reasonable: by (21), if $\alpha > 0$ the differential shearing near the MPEP is such as to enhance the likelihood of motion away from the MPEP in order to overcome the resistance of the drift field.

IV. SHORT-TIME BEHAVIOR AND UNSUCCESSFUL ESCAPES

We turn to the short-term dynamics of our model, and consider the trajectories followed by the particle in the exponentially many unsuccessful escape attempts which precede the final successful escape along the MPEP. The situation in the presence of detailed balance is well known. An unsuccessful escape attempt, defined as a sample path which leaves the diffusion-dominated region of size $O(\epsilon^{1/2})$ surrounding the stable point S, with high probability follows a trajectory moving antiparallel to the drift. The return path follows a deterministic trajectory satisfying $\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x})$. This symmetry is a consequence of time reversibility.

If detailed balance is absent, the instanton trajectories (i.e., the classical trajectories with nonzero momentum and zero energy, as determined by the Wentzell-Freidlin Hamiltonian, emanating from the stable point) serve as the most likely unsuccessful escape paths. This can be seen in several ways. The Wentzell-Freidlin Hamiltonian (7) is dual to the Onsager-Machlup Lagrangian

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2D_x}|\dot{x} - u_x|^2 + \frac{1}{2D_y}|\dot{y} - u_y|^2. \tag{31}$$

The probability that a sample path will be close to any specified trajectory $\mathbf{x}^*(t)$, $0 \le t \le T$, should to leading order fall off exponentially in ϵ, with a rate constant equal to the integral of the Lagrangian along $\mathbf{x}^*$. This integral is minimized when $\mathbf{x}^*$ is a *classical* trajectory, and it is easily seen that minimizing the integral over transit time T, for fixed end points $\mathbf{x}^*(0)$ and $\mathbf{x}^*(T)$, selects out the classical trajectories of zero energy.

There are in general many such trajectories, including the deterministic trajectories which simply follow the drift. (For them, L is identically zero.) We have adopted the field-theoretic nomenclature of Coleman [32], according to which the most likely exiting trajectories are called "instantons," and the return trajectories are anti-instantons. A careful treatment, using functional-integral methods, shows that the most likely trajectories, i.e., the local minima of the action functional, consist of any number of (pieces of) instanton trajectories, each followed by the corresponding anti-instanton trajectory: the relaxation toward the stable point S provided by the deterministic dynamics. Our nonequilibrium potential $W(x, y)$ is simply the classical action of the instanton trajectory terminating at (x, y).

Graham and others [26] have stressed the importance of the nonequilibrium potential in determining the long-term dynamics or MFPT, as well as the MPEP. However, its importance in short-term dynamics has seldom if ever been clearly enunciated. The fact of the matter is this: If the system is observed to be in some internal state S' far from the stable state S, with high probability it reached S' by following an instanton trajectory, and will return to S by following an anti-instanton trajectory. This applies to states S' which are outside the diffusion-dominated zone of size $O(\epsilon^{1/2})$ surrounding S, and the phrase "with high probability" can be given a quantitative meaning in the weak-noise limit. In the absence of detailed balance the outward instanton trajectories are not antiparallel to the inward anti-instanton trajectories, and the resulting closed loops contain nonzero area. This is a consequence of time irreversibility.

Figure 2 illustrates this phenomenon. If $D_x = D_y = 1$ and the drift field $\mathbf{u}$ is given by (21) and (22) with $\alpha = 0$, detailed balance is absent. Though the nonequi-

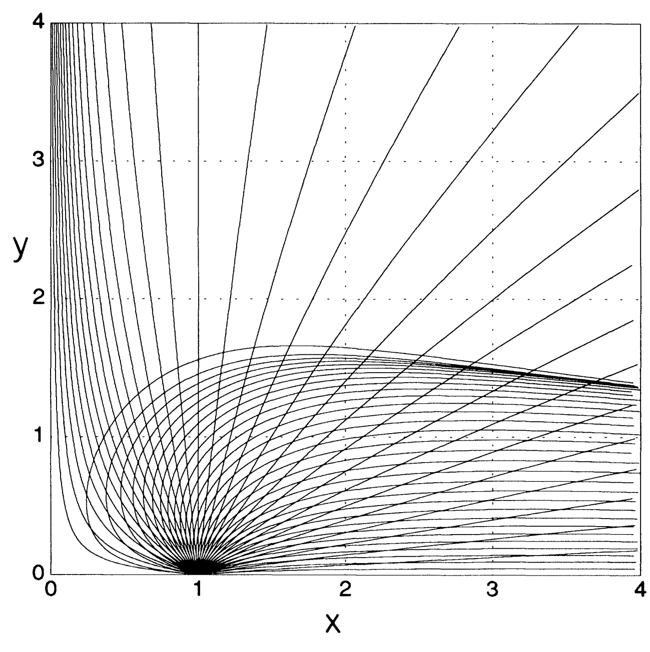

FIG. 2. Typical instanton and anti-instanton trajectories for the drift field specified by Eqs. (21) and (22), with $\alpha = 0$. The two families are superimposed: the anti-instanton trajectories are largely straight, but the instanton trajectories curve strongly to the right. The focus mentioned in the text occurs to the right. Diffusion here is isotropic; $D_x = D_y = 1$.

librium potential cannot be computed explicitly except along the x axis, the instanton and anti-instanton trajectories are easily computed numerically. Typical trajectories are shown. That the x-axis instanton trajectory (i.e., the MPEP) is atypical, being directly antiparallel to the drift, is in part a consequence of the symmetry of our model. It is also a consequence of the fact that by (8) and (9), we are assuming $\partial u_y/\partial x = \partial u_x/\partial y$ to hold along the MPEP. Within the WKB tube of width $O(\epsilon^{1/2})$ about the MPEP, to high accuracy $\mathbf{u}$ is irrotational and detailed balance holds. However, the small deviations from detailed balance due to differential shearing can, as we have seen, prevent transverse fluctuations from being in local thermal equilibrium.

Figure 2 also illustrates the phenomenon of focusing: several of the instanton trajectories displayed intersect each other, though not along the MPEP. Due to such intersections (which typically form *caustics* [33, 34], or singular surfaces of codimension unity) the computation of the nonequilibrium potential W will in general require a minimization over trajectories which are *piecewise classical* (with zero energy) rather than classical. Some preliminary investigations of this effect have been made by Graham and Tél [35], but it is not yet clear how to handle foci appearing along the MPEP. In our model it is easily checked that f_2 being driven through zero to $-\infty$ is the sign of a focus along the MPEP, in fact of a cusp catastrophe [33]. The appropriate extensions to the WKB approximation are now under study.

Note that though our instanton and anti-instanton trajectories are incident on the stable point S and/or the saddle point H, the portion of any trajectory within an $O(\epsilon^{1/2})$ distance of either equilibrium point is without physical significance. On this length scale diffusion dominates in the sense that the particle can diffuse from any point to any other within $O(1)$ time.

This sheds light on the seeming paradox of the trajectories having infinite transit time. Since $\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x})$ for anti-instanton trajectories an infinite amount of time is needed to reach S; similarly an infinite amount of time is needed for the instanton trajectories to emerge from S. The physical escape trajectories, both successful and unsuccessful, should be viewed as emerging from the diffusion-dominated zone rather than from S itself. So, for example, any unsuccessful escape trajectory directed along the x axis will have transit time

$$|\lambda_x(S)|^{-1}\ln(1/\epsilon^{1/2}) + O(1). \tag{32}$$

The transit time of the return path, i.e., the corresponding anti-instanton trajectory, will be the same. Similarly, the amount of time needed for the final, successful escape trajectory to approach H will be

$$\lambda_x(H)^{-1}\ln(1/\epsilon^{1/2}) + O(1). \tag{33}$$

In all

$$[|\lambda_x(S)|^{-1} + \lambda_x(H)^{-1}]\ln(1/\epsilon^{1/2}) + O(1) \tag{34}$$

time units will be required for the MPEP to be traversed in full during the successful escape.

We see that there are two time scales: the exponentially large MFPT and the logarithmic time scale on which escape attempts occur. In the weak-noise limit the latter is very brief compared to the former; the number of unsuccessful escape attempts grows nearly exponentially. The successful escape, when it finally occurs, will on the MFPT time scale occur almost instantaneously; this justifies the term "instanton."

V. SUMMARY AND CONCLUSIONS

We have seen that even in the absence of detailed balance, the weak-noise MFPT asymptotic behavior of a nonlinear system with a point attractor can readily be computed. There is no simple expression for the preexponential factor in the asymptotic behavior, such as that given by the Eyring formula. Rather, it follows by integrating the differential equations (13) and (14) along the MPEP. This technique clarifies the new phenomena that can occur, such as the formation of focusing singularities due to differential shearing along the MPEP. The effects of these singularities on the MFPT asymptotic behavior will be treated in the future.

Our treatment makes it clear that the time irreversibility present in systems without detailed balance manifests itself even on the shortest time scales. It is well known that in such systems stationary states, and the quasistationary state we employ to compute the MFPT asymptotic behavior, are characterized by a global circulation of probability. However, the circulation discussed in Sec. IV differs from the conventional sort [36] in that it occurs locally, at the level of *individual* unsuccessful escape attempts. Recognition of this point is essential for a proper computation of the MFPT asymptotic behavior.

In this paper we have treated the two-dimensional case on account of its simplicity, but our treatment generalizes to higher dimensions. Curved MPEP's, diffusion tensors whose principal axes are not aligned with the MPEP, and nonconstant diffusion tensors can all be treated by appropriate extensions of the techniques presented here. In higher-dimensional models, or models with curved MPEP's, the Riccati equation (13) must be replaced by a *matrix* Riccati equation. This extension is related to a standard result of stochastic control theory [37]: the effects of perturbing about optimal trajectories, obtained by solving a Hamilton-Jacobi equation, can be computed by solving a matrix Riccati equation.

Most studies of the overdamped escape problem have dealt with time-reversible stochastic models, with detailed balance. This is a reflection of the origins of the escape problem in statistical mechanics, where nonlinear dynamics are usually derived from a potential. In broader applications of stochastic modeling, which include engineering as well as the biological and social sciences, there is little reason to expect time reversibility. Our approach should prove useful in the wider context.

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[1] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[2] *Theory of Noise-Induced Processes in Special Applications*, edited by F. Moss and P. V. E. McClintock, Noise in Nonlinear Dynamical Systems Vol. 2 (Cambridge University Press, Cambridge, 1989).

[3] P. Hänggi, P. Talkner, and M. Borkovec, Rev. Mod. Phys. **62**, 251 (1990).

[4] R. S. Maier and D. L. Stein, Phys. Rev. Lett. **69**, 3691 (1992).

[5] D. L. Stein, R. G. Palmer, J. L. van Hemmen, and C. R. Doering, Phys. Lett. A **136**, 353 (1989).

[6] J. Ross, K. L. C. Hunt, and P. M. Hunt, J. Chem. Phys. **96**, 618 (1992).

[7] R. Nelson, J. Assoc. Comput. Mach. **34**, 661 (1987).

[8] J.-T. Lim and S. M. Meerkov, IEEE Trans. Commun. **35**, 1278 (1987).

[9] R. S. Maier, in *Proceedings of the 30th Allerton Conference on Communication, Control and Computing, Monticello, IL, 1992* (University of Illinois, Urbana, IL, 1992), pp. 674–681.

[10] W. Ebeling and L. Schimansky-Geier, in *Theory of Continuous Fokker-Planck Systems* (Ref. [38]), Chap. 8, pp. 279–306.

[11] M. Mangel, Theor. Population Biol. (to be published).

[12] T. Naeh, M. M. Kłosek, B. J. Matkowsky, and Z. Schuss, SIAM J. Appl. Math. **50**, 595 (1990).

[13] P. Talkner, Z. Phys. B **68**, 201 (1987).

[14] S. Glasstone, K. J. Laidler, and H. Eyring, *The Theory of Rate Processes* (McGraw-Hill, New York, 1941).

[15] B. Caroli, C. Caroli, B. Roulet, and J.-F. Gouyet, J. Stat. Phys. **22**, 515 (1980).

[16] R. Landauer and J. A. Swanson, Phys. Rev. **121**, 1668 (1961).

[17] J. S. Langer, Ann. Phys. (N.Y.) **54**, 258 (1969).

[18] Z. Schuss, *Theory and Application of Stochastic Differential Equations* (Wiley, New York, 1980).

[19] M. M. Kłosek-Dygas *et al.*, J. Chem. Phys. **90**, 1141 (1989).

[20] B. J. Matkowsky, A. Nitzan, and Z. Schuss, J. Chem. Phys. **88**, 4765 (1988).

[21] R. Landauer, Phys. Rev. A **12**, 636 (1975).

[22] R. Landauer, Helv. Phys. Acta **56**, 847 (1983).

[23] P. Talkner and P. Hänggi, Phys. Rev. A **29**, 768 (1984).

[24] D. Ludwig, SIAM Rev. **17**, 605 (1975).

[25] M. I. Freidlin and A. D. Wentzell, *Random Perturbations of Dynamical Systems* (Springer-Verlag, Berlin, 1984).

[26] R. L. Graham, in *Theory of Continuous Fokker-Planck Systems* (Ref. [38]), Chap. 7, pp. 225–278.

[27] R. Kupferman, M. Kaiser, Z. Schuss, and E. Ben-Jacob, Phys. Rev. A **45**, 745 (1992).

[28] M. V. Day, Stochastics **20**, 121 (1987).

[29] P. Talkner and D. Ryter, in *Proceedings of the 7th International Conference on Noise in Physical Systems, Montpellier, 1983* (North-Holland, Amsterdam, 1983), pp. 63–66.

[30] M. Mangel and D. Ludwig, SIAM J. Appl. Math. **33**, 256 (1977).

[31] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965).

[32] S. Coleman, in *The Whys of Subnuclear Physics*, edited by A. Zichichi, Proceedings of the International School of Physics "Enrico Fermi," Erice, 1977 (Plenum, New York, 1977), pp. 805–916. A recent study based on the instanton picture is A. J. Bray and A. J. McKane, Phys. Rev. Lett. **62**, 493 (1989).

[33] L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).

[34] V. A. Chinarov, M. I. Dykman, and V. N. Smelyanskiy, Phys. Rev. E **47**, 2448 (1993).

[35] R. Graham and T. Tél, Phys. Rev. A **33**, 1322 (1986).

[36] R. Landauer, J. Stat. Phys. **53**, 233 (1988).

[37] W. H. Fleming and R. W. Rishel, *Deterministic and Stochastic Optimal Control* (Springer-Verlag, Berlin, 1975).

[38] *Theory of Continuous Fokker-Planck Systems*, edited by F. Moss and P. V. E. McClintock, Noise in Nonlinear Dynamical Systems Vol. 1 (Cambridge University Press, Cambridge, 1989).